Author: Marek Nedoma

Study programme: Mechanical Engineering

Field of study: Energy and Process Engineering

Supervisor: Professor Jan Hrdlička

CTU CZECH TECHNICAL UNIVERSITY IN PRAGUE

Department of Energy Engineering

Low-temperature adsorption for post-combustion CO_2 capture from fossil fuel combustion

Objective. *This thesis investigated the viability of low-temperature adsorption process for post-combustion CO_2 capture (PCC) using process simulation. First, a literature review was made to identify process configuration and potential applications. Then, a simplified MATLAB-based model was created for breakthrough experiments prediction and initial process design, and later modified to assess the performance and economy of a 4-step vacuum-swing adsorption (VSA) with zeolite 13X for district-scale cogeneration and heat plant (CHP). Consequently, a flue gas cleaning process downstream from the CHP was proposed and economically evaluated.*

Introduction

Aims

- **Process**: physical adsorption on solid adsorbents.
- **Application**: PCC in fossil fuel-fired emission sources.

WHY? (1) *smooth transition to renewables is not immediate.* (2) *alternatives to amine-absorption are critically needed.*

Methodology

1. **In-depth literature review**: process configuration & application.
2. **Mathematical modelling**: adsorption phenomena & 4-step VSA.
3. **Process design**: VSA PCC process downstream from the CHP.
4. **Economic assessment**: individual PCC chain processes.

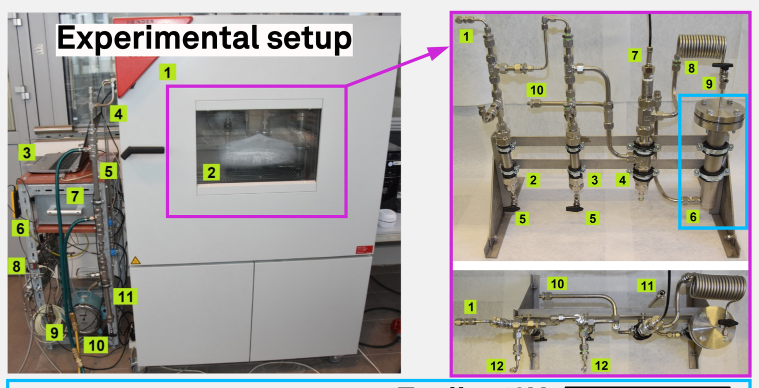
Literature review

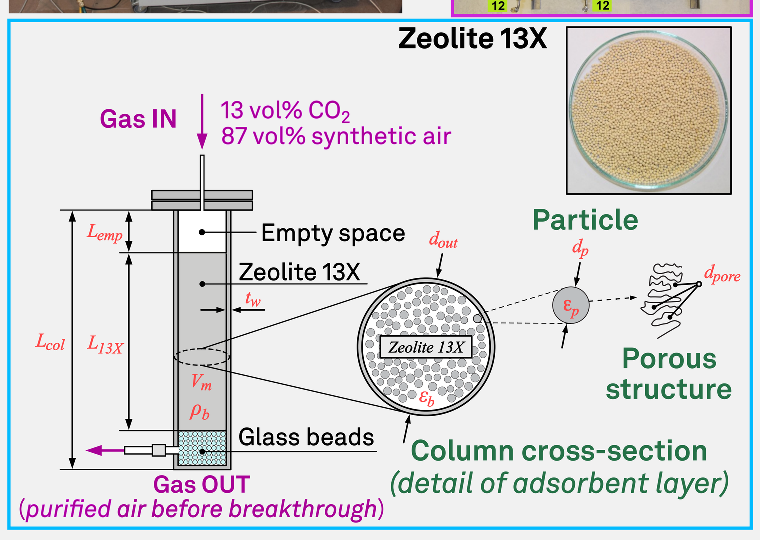
- **Findings**: **process**: basic 4-step VSA, **adsorbent**: zeolite 13X, **approach**: theoretical *via* mathematical modelling (*MATLAB*).
- **Research gaps**: adsorption for PCC in a small-scale power plants with CO_2-lean emission (*e.g.* natural gas).

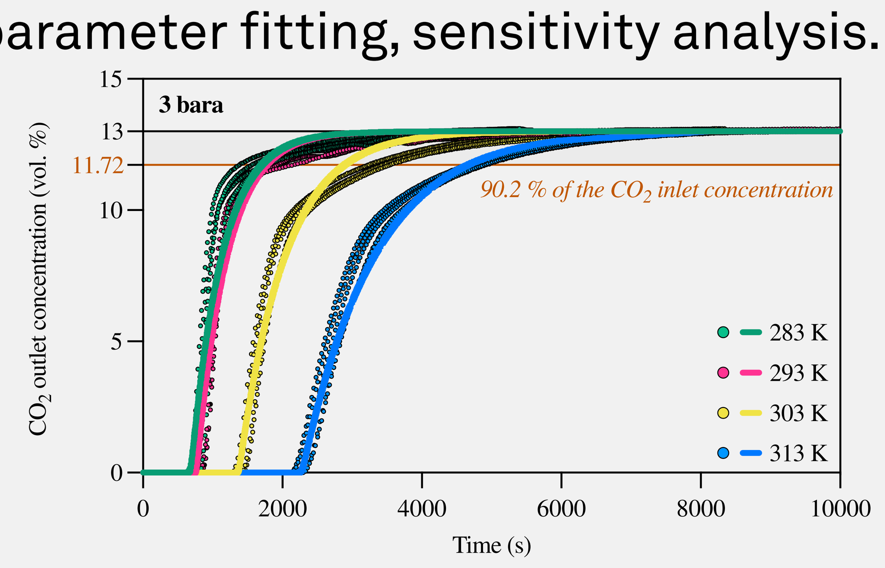
Adsorption phenomena modelling

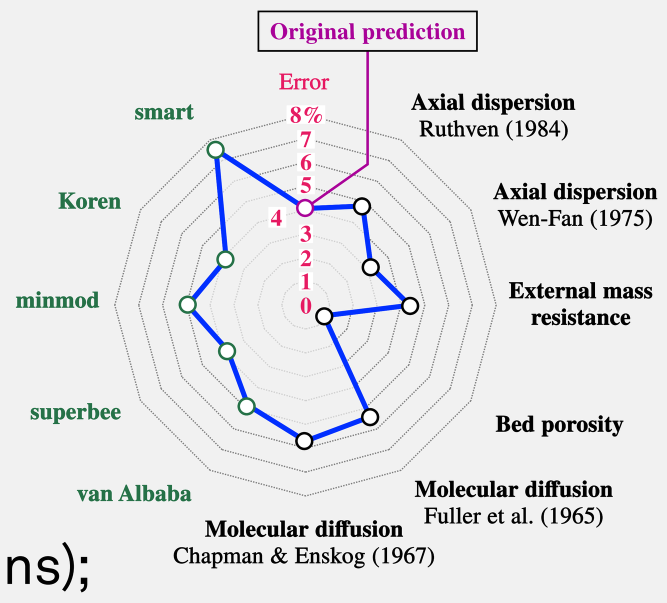
Breakthrough experiments

- **Approach**: model verification, parameter fitting, sensitivity analysis.







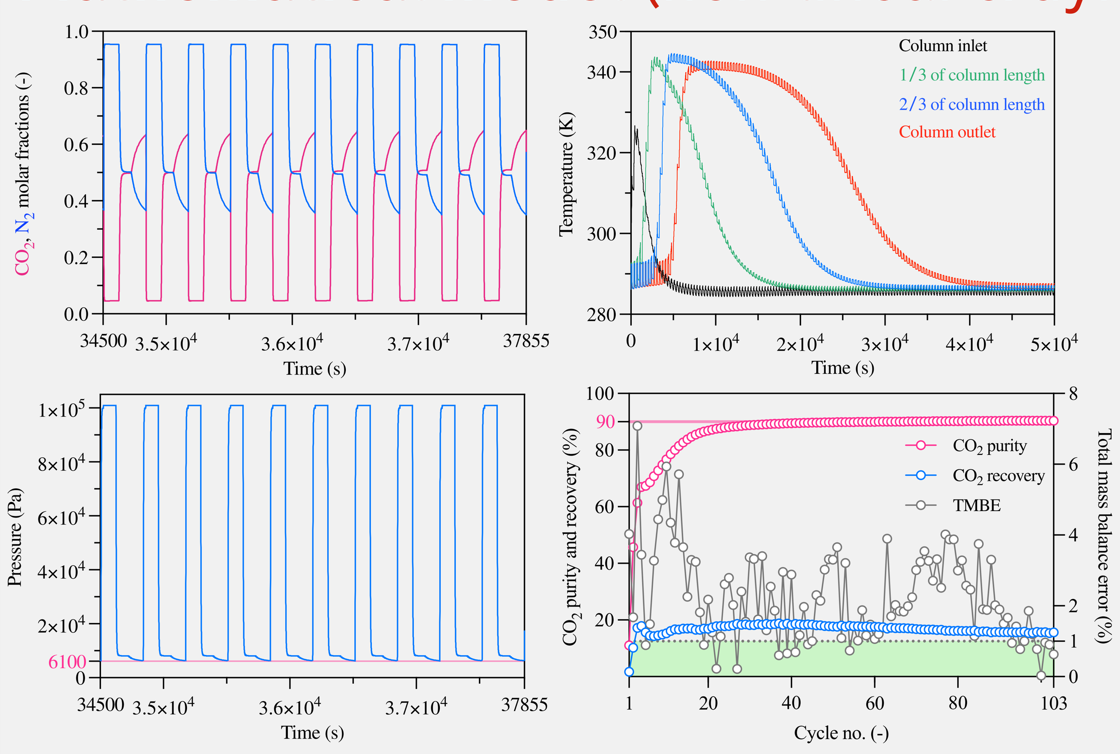


Initial VSA process design

- **Results**: **column size**: 2 × 1 m (8 columns); **pressure range**: 1 - 0.13 bara; **interstitial velocity**: 1.9 m.s^{-1}.

4-step VSA modelling

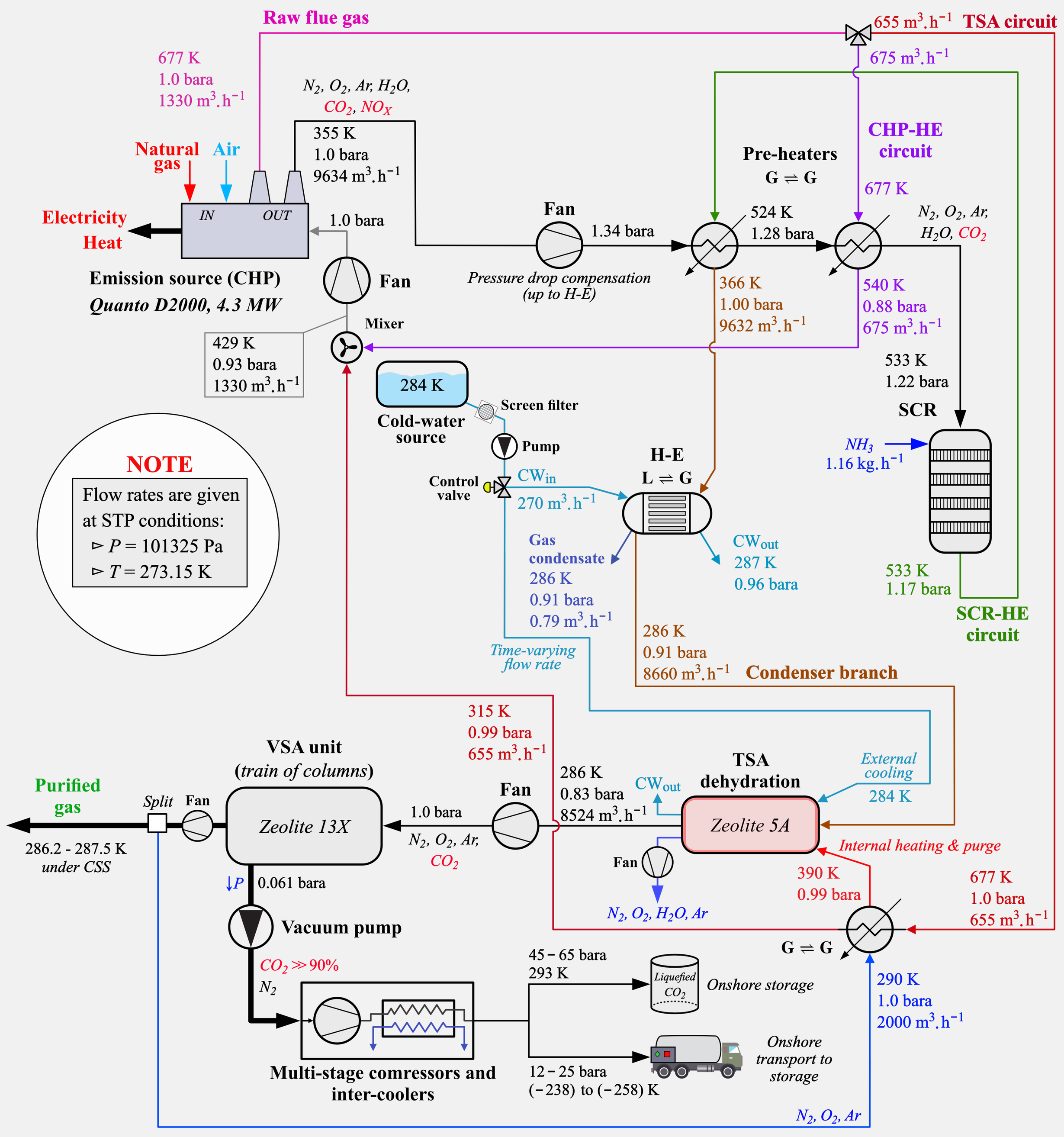
Mathematical model (non-linear & dynamic, FVM)



VSA

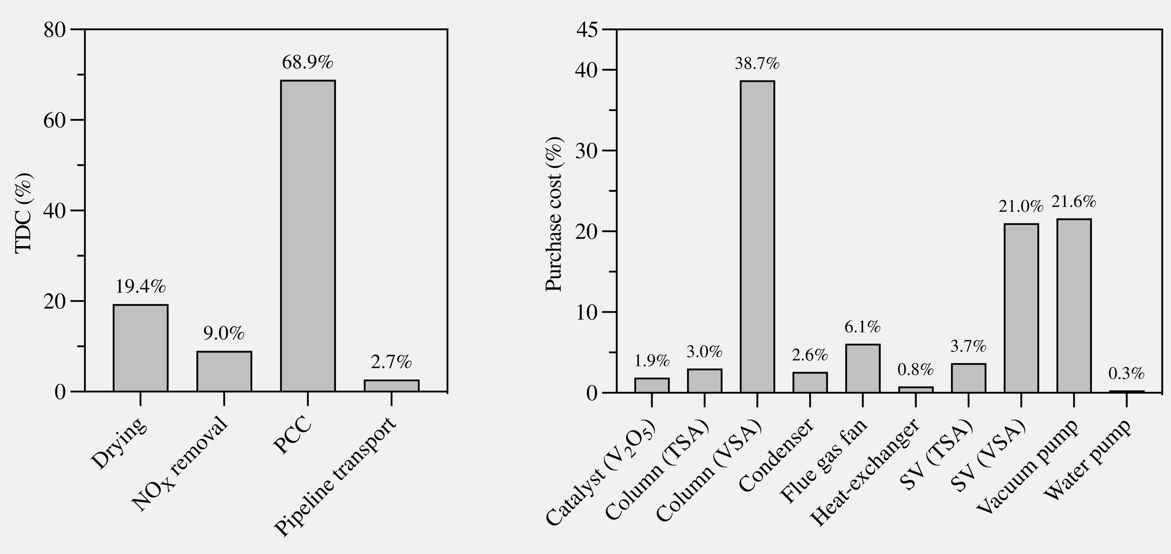
- **System size**: 5 columns in 3 trains (16.8t of 13X)
- **Configuration**: 360 s per cycle, evacuation and intermediate pressures of 0.081 and 0.061 bara
- **Performance**: CO_2 purity and recovery: 90.4 %, 15.6 %

PCC process design (ready-to-operate)



- **Core systems**
  - SCR-deNO$_X$
  - two-step dehydration
    - 1° condenser
    - 2° TSA (zeolite 5A)
  - 4-step VSA for PCC
- **Auxiliary components**
  - fans
  - heat-exchangers
  - pumps
- **CHP**
  - 4.3 MW, 9000 m^3.h^{-1}, 6.4 % CO_2 (+ NO$_X$, CO)
- **Calculations**
  - *MATLAB*
  - *Aspen Plus*
  - Empirical design

Economic assessment (PCC process chain)



- **Results**: PCC is the most expensive process: ~70 % of the total process chain direct purchase costs.

Conclusions & Outlook

- **Accomplished objectives**

(1) Development of a simplified mathematical model of adsorption phenomena, with subsequent analysis of the numerical approach and balance equations supported by experimental data to verify model robustness and reliability, and its application for process design.

(2) Development of a complex non-linear dynamic mathematical model of 4-step VSA process, enabling simulation of various scenarios for different process parameters and configurations, and its application to experimental and theoretical studies.

(3) Design of adsorption PCC system integrated into an urban-scale energy system, including general economic assessment.

- **Outlook**: **model**: experimental validation, VSA steps and gas species addition, process optimiser implementation, and neural network exploration.

Author's publications

1. Nedoma, M., & Netušil, M. (2021). Chemical Engineering Transactions, 88, 421-426.
2. Nedoma, M., Netušil, M., & Ditl, P. (2022). Chemical Engineering Transactions, 94, 283-288.
3. Nedoma, M., Staf, M., & Hrdlička, J. (2022). *Acta Polytechnica*, 62(3), 370385.
4. Nedoma, M., Netušil, M., & Hrdlička, J. (2023). Integration of adsorption based post-combustion carbon dioxide capture for a natural gas-fired combined heat and power plant. *Accepted for publication in Fuel (ISSN 0016-2361) on 29. 07. 2023.*

Czech Technical University in Prague, FME

Department of Energy Engineering

Technická 4, 160 00 Prague 6 - Dejvice

Czech Republic